



Transient Catalytic Combustor Model With Detailed Gas and Surface Chemistry

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Abstract

In this work, we numerically investigate the transient combustion of a premixed gas mixture in a narrow, perfectly-insulated, catalytic channel which can represent an interior channel of a catalytic monolith. The model assumes a quasi-steady gas-phase and a transient, thermally thin solid phase. The gas phase is one-dimensional, but it does account for heat and mass transfer in a direction perpendicular to the flow via appropriate heat and mass transfer coefficients. The model neglects axial conduction in both the gas and in the solid. The model includes both detailed gas-phase reactions and catalytic surface reactions. The reactants modeled so far include lean mixtures of dry CO and CO/H₂ mixtures, with pure oxygen as the oxidizer. The results include transient computations of light-off and system response to inlet condition variations. In some cases, the model predicts two different steady-state solutions depending on whether the channel is initially hot or cold. Additionally, the model suggests that the catalytic ignition of CO/O₂ mixtures is extremely sensitive to small variations of inlet equivalence ratios and ppm levels of H₂.

I. Introduction

Recently, catalytic combustion in narrow channels has received renewed interest in the research community owing to the pursuit of micro combustion devices. Modeling the flow of fuel and oxidizer through a narrow channel can employ a wide variety of assumptions and boundary conditions. Considering an interior channel of a monolith reactor allows the use of adiabatic boundary conditions in the radial direction, whereas a single tube reactor requires an appropriate heat flux boundary condition, a complication not included in the present research. With regard to flow field, Raja, et al. (2000) compares the various flow modeling assumptions including Navier-Stokes, boundary-layer, and plug-flow and offers valid ranges for each model based on Reynolds number. While detailed flow-field models such as Navier-Stokes are more universally valid, they are also more computationally expensive, especially in non-circular channels in which the detailed flow field is three-dimensional.

Steady-state catalytic combustor models date back to the steady-state, isothermal plug-flow model of Khitrin and Solov'yeva (1958). T'ien (1981) was one of the first to model the transient behavior of a catalytic combustor. The model, which assumes a quasi-steady gas phase and transient solid phase, successfully predicted some transient characteristics of catalytic combustors. Also, this model could apply to a variety of cross-sectional geometries as a reasonable approximation. Later work by Tien and T'ien (1992) included a non-isothermal porous catalytic layer with a full transient model and identified kinetically and diffusionally controlled regions. Wanker et al. (2000) investigated the transient behavior of a single-channel monolith including the non-isothermal reaction/diffusion in a wash coat catalytic layer using FLUENT. Most recently, Deutschmann's group (Schwiedernoch, et al. 2003) numerically modeled the transient behavior of methane oxidation in a catalytic monolith.

The gas-phase and surface chemistry models range from simple global reactions (T'ien 1981 and Wanker, 2000) to detailed, multi-step chemistry (Bond et al., 1996, Maruta et al., 2002, and Schwiedernoch, et al. 2003). Detailed homogeneous chemical mechanisms are readily available in the literature for many fuels. Heterogeneous mechanisms are increasingly becoming available (e.g. Deutschmann et al. 1996).

In this paper, we investigated the transient behavior of an adiabatic catalytic channel. By incorporating more recent detailed chemical mechanisms, we improved upon the model of T'ien (1981), which is numerically attractive because of its relative simplicity and applicability to a wide variety of channel geometries. Owing to the stiff nature of the resulting system of ordinary-differential algebraic equations, however, we required more complex numerical methods than the original Runge-Kutta scheme to solve the problem efficiently. The reactants modeled so far include lean CO and CO/H₂ mixtures in pure

oxygen. We computed cases showing catalytic ignition starting from cold initial condition and combustor response to inlet condition variations.

II. Model Description

The present numerical model is based on the original model of T'ien (1979, 1981). The model is of a single channel (solid platinum or substrate with platinum washcoat) through which passes a mixture of fuel, oxidizer, and optional inert. The combustion process considers both detailed gas phase and surface reactions. There is negligible pressure drop along the channel and the gas is ideal. The transient combustor time-lag is from the thermal inertia of the solid. The gas-phase model (Equations 1-3) is quasi-steady relative to the transient solid (Equation 5) owing to the significantly longer heat-up times of the solid (~sec) compared with the residence times of the gas in the channel (~ msec). In the gas-phase equations, heat and mass diffusion in the axial direction are neglected because the Peclet number based on typical gas velocities is much greater than unity.

Bulk temperatures, assuming no lateral gradients, describe the solid and gas along the channel. The formulation of the gas-phase energy equation (Equation 2) accounts for variable specific heats. There is convective heat transfer perpendicular to the flow. For the computed cases, we use a Nusselt number for developing flow in an isothermal circular tube. At the entrance, the heat-transfer coefficient is the stagnation-point value (see T'ien 1981 for details). To a reasonable approximation, this model is applicable to a variety of cross-sectional geometries typically seen in catalytic monoliths (e.g. see Figure 1). For non-circular geometries, hydraulic diameter can be used to evaluate the Nusselt number.

There are two values of gas-phase species, a bulk flow value and a value adjacent to the catalytic surface (Equation 3). Lateral (i.e. perpendicular to the flow) mass transfer coefficients come from the heat transfer coefficients using the analogy of heat and mass transfer (Incropera and DeWitt, 1990). The values of the gas-phase species adjacent to the catalytic surface come from a balance between the lateral mass transfer and the adsorption/desorption of species on the catalytic surface (Equation 4). Transport properties are calculated at the average temperature and mass fraction of the surface and bulk at each axial location.

The heat-transfer rate between the gas and solid is the dominant mode of heat transfer, thus we neglect heat conduction in the axial direction. The outside of the tube is perfectly insulated. The model of the catalytic reactions along the inner portion of the channel wall accounts for varying surface coverage of adsorbed species (Equation 6). The model assumes that the number of active surface sites, Γ , is constant (Equations 6 and 7).

For this paper, we consider both CO (dry) and CO/H₂ mechanisms and track the following species: H₂, H, O₂, O, OH, H₂O, HO₂, H₂O₂, CO, CO₂, HCO, Pt(s), H(s), H₂O(s), OH(s), CO(s), CO₂(s), C(s), and O(s). The heterogeneous reactions account for species adsorption, surface reactions, and desorption (Equation 8). The "(s)" nomenclature denotes species adsorbed to the surface while the symbol Pt(s) denotes vacant sites of the platinum surface. The chemical mechanisms come directly from the literature (e.g. Yetter, et al. 1991 for homogeneous reactions and Deutschmann, et al. 1996 for heterogeneous reactions) and account for only the species required. For example, no hydrogen species are accounted for when modeling pure dry CO oxidation.

Gas Phase Equations

Mass conservation:

$$\rho u A = \text{constant} \quad (1)$$

Energy conservation:

$$\rho u A \left(\bar{C}_p \frac{\partial T}{\partial x} + \sum_{k=1}^{K_g} h_k \frac{\partial Y_k}{\partial x} \right) \quad (2)$$

$$+ h_r S [T - T_s] = S \sum_{k=1}^{K_g} \dot{s}_k W_k h_k$$

Species conservation for species k:

$$\rho u A \frac{\partial Y_k}{\partial x} + \rho h_{Dk} S [Y_k - Y_{kw}] = \omega_k W_k A \quad (3)$$

Flux-matching at the surface:

$$\rho h_{Dk} (Y_k - Y_{kw}) = \dot{s}_k W_k \quad (k=1 \dots K_g) \quad (4)$$

Surface and Solid Equations

Energy conservation:

$$\rho_s C_s A_s \frac{\partial T_s}{\partial t} - h_H S [T - T_s] = S \sum_{i=1}^{n_s} Q_i q_i \quad (5)$$

Rate of change of surface site fractions:

$$\frac{\partial Z_k}{\partial t} = \frac{1}{\Gamma} \dot{s}_k \quad (k = 1 \dots K_s) \quad (6)$$

Site fraction conservation:

$$\sum_{k=1}^{K_s} Z_k = 1 \quad (7)$$

Chemistry Expressions

$$\dot{s}_k = \sum_{i=1}^{n_s} \nu_{ki} q_i \quad (8)$$

$$\omega_k = \sum_{i=1}^{n_g} \nu_{ki} q_i \quad (9)$$

$$q_i = k_{fi} \prod_{k=1}^K [X_k]^{v'_{ki}} - k_{ri} \prod_{k=1}^K [X_k]^{v''_{ki}} \quad (10)$$

$$[X_k] = \frac{\rho Y_{k,W}}{W_k} \text{ gas species / surface reactions} \quad (11)$$

$$[X_k] = \frac{\rho Y_k}{W_k} \text{ gas species / bulk reactions} \quad (12)$$

$$[X_k] = \frac{\Gamma Z_k}{\sigma_k} \text{ surface species concentration} \quad (13)$$

Initial and Boundary Conditions

The gas-phase equations (1-3) require boundary conditions for the inlet temperature, velocity, and species. The transient equations (5 and 6) require initial conditions for surface temperature and site fraction distribution along the channel. The initial surface temperature was 300K for this work (except for cases utilizing previously computed steady-states as discussed below). For dry CO cases, CO occupied all available sites on a 300K surface (i.e. $Z_{CO(S)}=1$). For CO/H₂ mixtures, however, we found that integration was difficult if we specified a single species to occupy all the available sites as an initial condition. Thus for CO/H₂ mixtures, the initial surface site fractions came from steady-state results at 300K. We obtained these initial conditions by running our program in an isothermal mode until the surface site fractions reached a steady-state. The initial values of the gas-phase species adjacent to the wall came from solving Equation 4 before beginning the time integration.

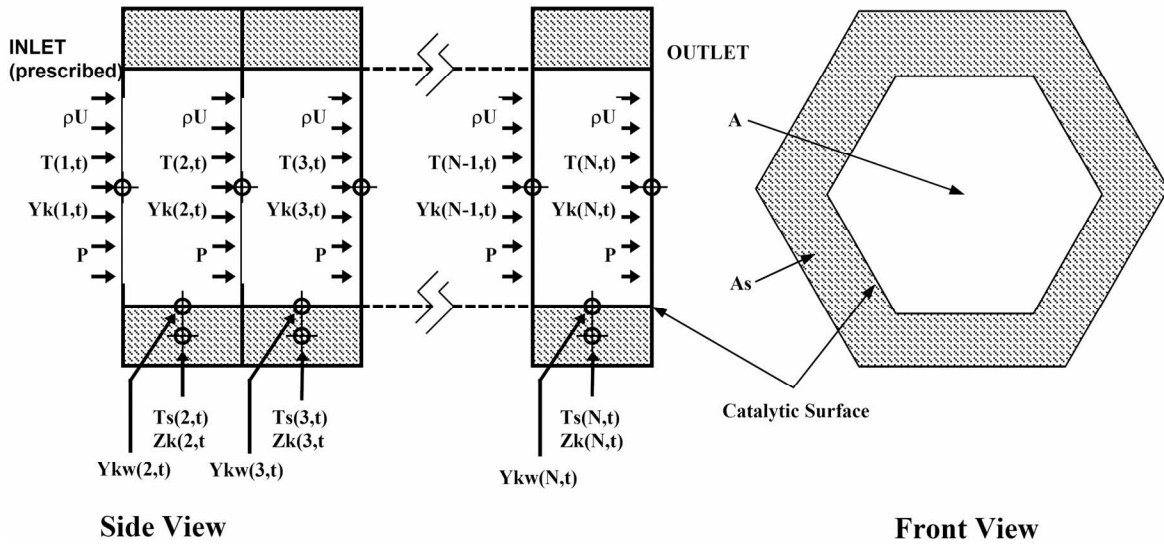


Figure 1. Discretized catalytic combustor channel. The cross-section (front view) can be extended to non-axis symmetric cases (as shown) because of the simplifications in the model.

Solution Procedure

Equations 1-13 form a series of coupled differential and algebraic equations. The assumption of a quasi-steady gas phase and of a thermally-thin solid simplify the solution procedure. The gas-phase ordinary differential-equations (2 and 3) are integrated analytically across spatially uniform control volumes which divide the channel (Figure 1). This integration results in algebraic relations for the bulk gas-phase values downstream (e.g. $T[2,t]$, $Y_K[2,t]$) dependent on the upstream values ($T[1,t]$, $Y_K[1,t]$) and implicitly solved surface values ($Ts[2,t]$, $Y_{K,W}[2,t]$, and $Z_K[2,t]$). Thus, the system of equations are reduced to ordinary differential (5,6) and algebraic (1,4,7 and analytically integrated 2,3) equations. The detailed chemistry (equations 8-12) make the series of equations stiff and thus require special solution procedures. We utilize the publicly available DASSL code (Brenan, et al. 1996) to integrate in time. The integration begins at the most upstream control volume. Since solution components do not depend on downstream values, the solution proceeds completely in time at this single axial location before proceeding to the next downstream location. The solution components, which are output in discrete time intervals, become the upstream values for each subsequent integration. The upstream components are continually interpolated

for intermediate time-steps required in the solution. DASSL chooses an appropriate initial time step but a maximum time step (typically half of the output interval) is enforced to allow for accurate temporal interpolation.

III. Computed Results

Reactant gas at 600K enters the initially 300K channel at 2 m/s and 1 atmosphere pressure. The channels cross-sectional dimensions are in the nomenclature. The channel is 1 cm long resulting in a cold-flow residence time of 5 ms. There are 250 uniform control volumes along the channel for the spatial integration. For the purposes of this paper, we consider very lean CO mixtures in pure O₂ environments. The inlet mass fraction of CO for each case is 0.05 or less (equivalence ratio, $\phi \leq 0.03$). The CO/H₂ cases have 10 ppm of H₂ added to the inlet stream. Full CO/H₂ chemistry (gas and surface reactions) increases computational time significantly. For the fuel/oxidizer mixtures in this study, however, only surface reactions release significant amounts of heat. The small amounts of H₂ are negligible for purposes of gas-phase chemistry but affect surface kinetics significantly. Therefore, we compare results with complete CO/H₂ surface chemistry only (i.e. neglecting gas phase chemistry) which increases the computational time only slightly compared to dry CO, but produces results virtually identical to the full chemistry for the computed cases. The initial surface site fraction distribution was 9.98×10^{-1} , 1.71×10^{-3} , and 1.09×10^{-8} for CO(s), H(s), and Pt(s), respectively, with the remaining surface species appearing in only trace amounts.

Transient Results

Figure 2 shows the transient results for the case of $Y_{CO} = 0.04$ and $Y_{H_2} = 10$ ppm (balance O₂) where $\phi = 0.02388$. The results are for channel temperature, species, and site fraction profiles at 4 specific time intervals ($t = 0, 2\tau^*, 40\tau^*$, and $190\tau^*$, where τ^* is the characteristic channel heat-up time, ~ 1.6 sec. for our channel). Figure 2 shows that, as the incoming gas heats the solid surface, O(s) replaces CO(s) as the major surface constituent throughout the computation. Starting at about $t = 4\tau^*$ (not shown), some surface reactions occur at the inlet as indicated by a surface temperature greater than 600K. As the surface reaches about 750K, a sharp ignition appears at the rear of the channel and propagates in time to a fixed upstream location ($x = 0.45$ cm in this case). By $40\tau^*$, the conversion of CO is greater than 99.9% at the end of the channel. In steady-state, the surface temperature exceeds the adiabatic flame temperature (984K) by approximately 40K at the ignition front. The surface then exchanges heat with the gas and by $x = 0.86$ cm both are within 2K of the adiabatic flame temperature.

Steady-State Results

Figure 3 shows several steady state results for dry CO oxidation. The flow and channel parameters were identical to the previously described transient case. The graph shows surface temperature as a function of the cold flow residence time (L/U) based on inlet velocity. Various combinations of L and U produced the same steady-state results when plotted as a function of L/U . For $\phi = 0.0238, 0.0244$ (thin lines with symbols) and the $\phi = 0.0301$ (solid line) cases, the initial condition was a surface temperature of 300K with all surface sites initially occupied by CO ($Z_{CO(s)} = 1$). For the lowest equivalence ratio of 0.0238, an ignition front stabilizes near the end of the channel. Increasing the inlet equivalence ratio to 0.0244 moves the steady-state ignition front upstream near the inlet of the channel. Further increasing the inlet equivalence ratio to 0.0301 (solid blue line) results in the peak surface temperature occurring exactly at the inlet. The other two results in Figure 3 are again for the lower equivalence ratios (0.0238 and 0.0244) but use the steady-state results from the $\phi = 0.0301$ case as the initial condition. Physically, this is analogous to operating the channel in steady-state at $\phi = 0.0301$ and changing the inlet condition suddenly. The results show that a different steady-state occurs with this initial condition (hatched red and green lines for $\phi = 0.0238$ and 0.0244, respectively). The peak surface temperature in these cases occurs at the inlet of the channel. Further reducing the inlet ϕ to 0.018 (not shown) causes the reaction front to propagate out the end of the channel resulting in an isothermal gas and solid spanning the entire length of the channel in steady-state.

Figure 4 shows the influence of surface and gas-phase chemistry on the steady-state solid surface temperature profiles. The hatched line denotes a computation using dry CO chemistry while the solid line and symbols denote CO/H₂ chemistry with 10 ppm H₂ added to the inlet gas. The case shown with the solid line, which is also the same test shown in Figure 2, does not include gas-phase reactions. Figure 4 shows that adding 10 ppm of H₂ to the CO / O₂ mixture ($\phi = 0.0238$) moves the steady-state catalytic ignition front forward from 0.86 cm to 0.47 cm. Figure 4 shows that the surface chemistry is responsible for the shift in ignition fronts and that gas-phase reactions do not contribute at these temperatures. The steady-state profiles in Figure 4 reveal that the surface temperature leading up to the ignition front is approximately 40K hotter with the addition of 10 ppm of H₂. Examination of the species and reaction rate profiles (see Figure 2) reveal that almost all of the H₂ reacts (94% conversion) before ignition. Also, surface CO reaction rates (not shown) roughly double in the pre-ignition region with the addition of 10 ppm H₂.

IV. Discussion and Conclusions

We present a model of a transient catalytic combustor with detailed gas and surface chemistry. In the current work, we present select cases of an adiabatic catalytic channel using lean CO/H₂ and pure O₂ mixtures at an inlet temperature of 600K. For these conditions, the results show that surface reactions are the predominant source of heat release. The transient

nature of the model allows for the computation of system response to different initial conditions of the solid (e.g. temperature). The model predicts different steady-states depending on whether the channel is initially cold or hot (using a previous steady-state solution). For initially cold surfaces with sufficiently lean mixtures, a preheat length precedes an abrupt ignition front (Figure 3). For cases where the initial condition was a hot surface or for sufficiently rich mixtures, significant surface reactions begin at the inlet. This observation suggests that a pre-heated channel can effectively reduce the residence time required to completely convert lean CO/O₂ mixtures for the conditions in this work.

According to our results, catalytic ignition of lean CO and pure O₂ mixtures is extremely sensitive to inlet concentrations, in addition to the initial condition. Increasing the inlet equivalence ratio from 0.0238 to 0.0244 (which corresponds to increasing the inlet fuel mass fraction from 0.04 to 0.041) reduced the required residence time for ignition from 4.3 to 1.3 seconds (Figure 3). Similar reductions in residence time occurred with small additions (10 ppm) of H₂ (Figures 2 and 4).

The current model neglects axial conduction in the solid phase. In regions where the surface temperature variation is steep (such as the ignition front), the addition of axial conduction is likely necessary to predict actual temperature profiles. Adding axial conduction would allow heat to diffuse upstream thereby shifting and broadening the reaction zones. Nevertheless, the current model includes some of the essential physics required to predict the transient performance of catalytic micro-channels.

V. Nomenclature

Γ	- site density (2.7063×10^{-5} mol/m ² for Pt)	K	- total number of species ($K_s + K_g$)
ρ	- mass density of gas (kg/m ³)	n_g	- number of gas-phase reactions
ρ_s	- mass density of solid (21450 kg/m ³)	n_s	- number of surface reactions
τ^*	- Substrate heat-up time, see T'ien 1981 (~1.55 sec.)	N	- number of axial grid points (250)
v_{ki}	- net stoich. coeff., k th specie, i th reaction;	Q_i	- heat evolved from the i th reaction
v'_{ki}	- stoich. coeff., k th reactant specie, i th reaction	P	- pressure
v''_{ki}	- stoich. coeff., k th product specie, i th reaction	q_i	- rate of progress of the i th gas-phase reaction
ω_k	- k th gas-species production for gas reactions	\dot{S}_k	- net prod. rate of species k due to surface reactions
A	- channel flow area (5.027×10^{-7} m ²)	S	- circumferential length of channel cross section = πd
A_s	- solid cross-sectional area (2.827×10^{-7} m ²)	t	- time
\bar{C}_P	- mean gas specific heat at const. P (J / kg /K)	T	- bulk gas temperature
C_s	- solid specific heat (J / kg /K)	T_s	- solid temperature
L	- length of catalytic channel (1 cm)	U	- average (bulk) velocity of flow
h_k	- total enthalpy of species k	W_k	- molecular weight of species k
h_{Dk}	- convection mass transfer coefficient for species k in bulk mixture	x	- axial coordinate from channel inlet
h_T	- convection heat transfer coefficient	$[X_k]$	- molar concentration of species k
k_{fi}	- forward rate constant for the i th reaction	Y_k	- mass fraction of species k in the bulk mixture
k_{ri}	- reverse rate constant for the i th reaction	Y_{kw}	- mass fraction of species k at the wall
K_g	- number of gas-phase species	Z_k	- site fraction of surface species k
K_s	- number of surface species		

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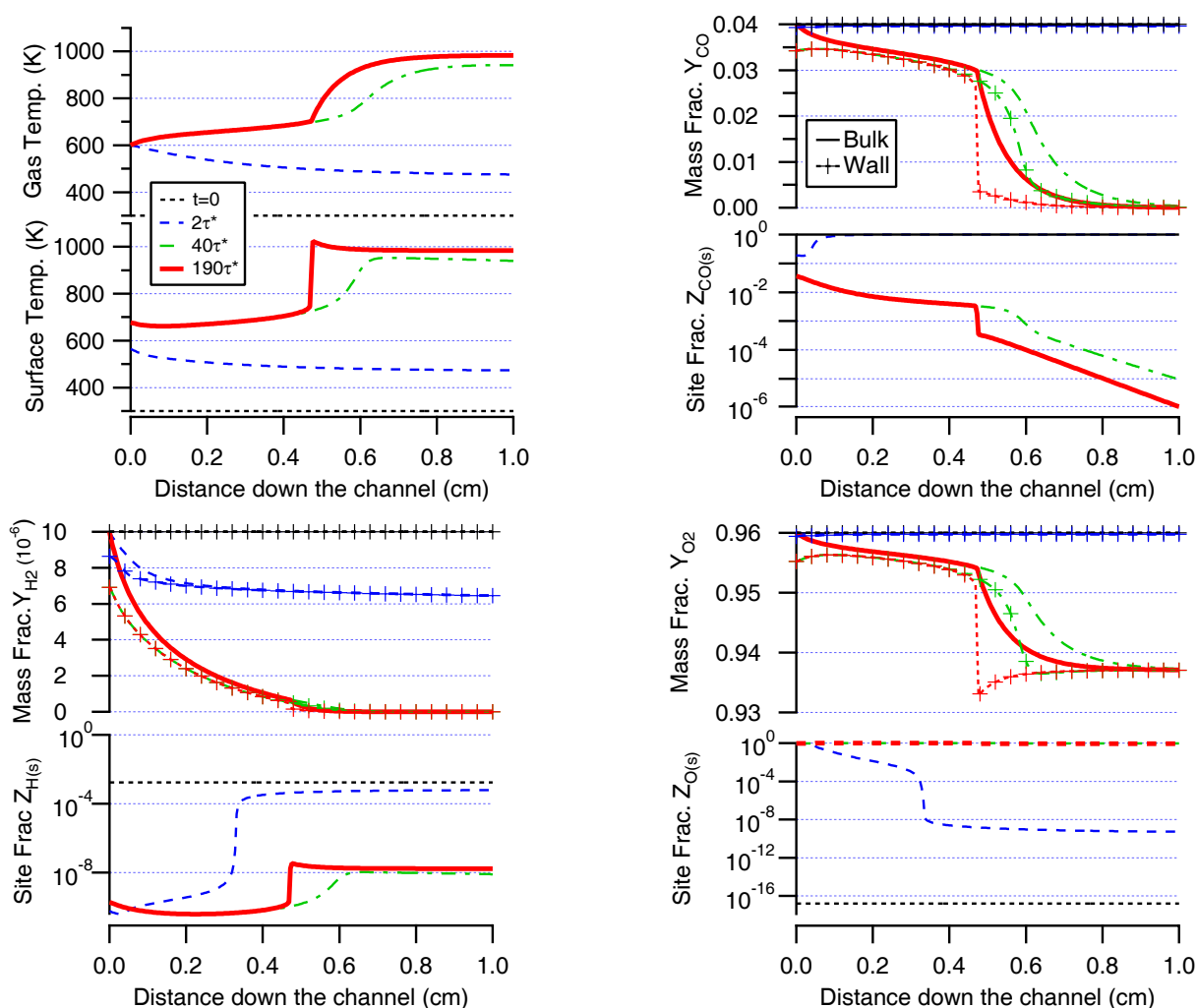


Figure 2. Select transient profiles (temperature, CO, H₂, and O₂) for the case of $\phi = 0.02388$ ($Y_{CO} = 0.04$, $Y_{H_2} = 10$ ppm, balance O₂) from $t = 0$ to $t = 190\tau^*$ (~295 seconds) which is essentially steady-state.

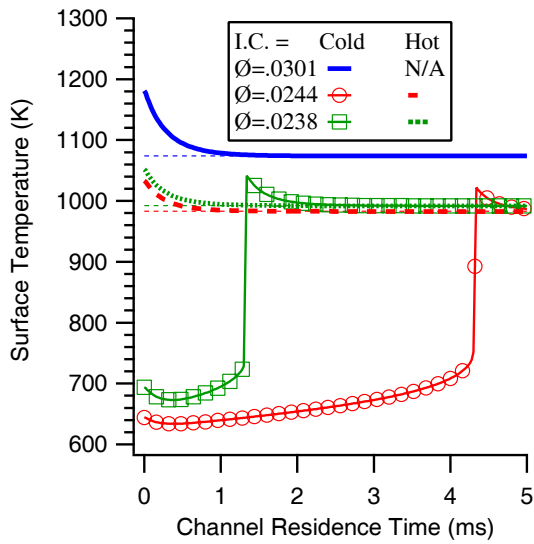


Figure 3. Plots of 2 separate steady-states achieved using different initial surface conditions. The channel residence time is computed using cold flow conditions (i.e. based on inlet velocity).

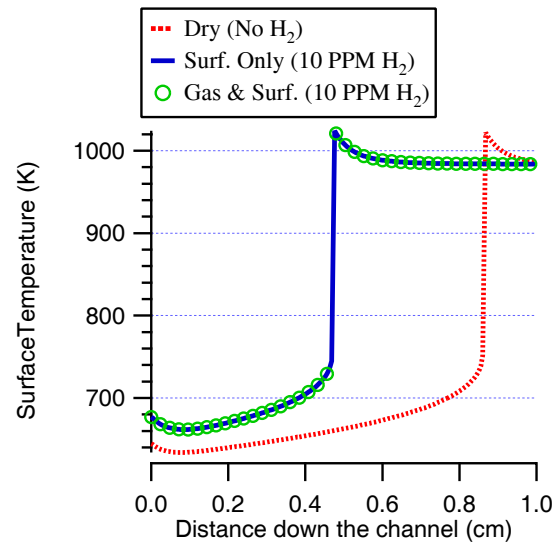


Figure 4. Effect of H₂ addition on catalytic ignition of a CO/O₂ system ($\phi = 0.0238$). The “Surf. Only” case is the same test shown in Figure 2.

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13. ABSTRACT (Maximum 200 words) In this work, we numerically investigate the transient combustion of a premixed gas mixture in a narrow, perfectly-insulated, catalytic channel which can represent an interior channel of a catalytic monolith. The model assumes a quasi-steady gas-phase and a transient, thermally thin solid phase. The gas phase is one-dimensional, but it does account for heat and mass transfer in a direction perpendicular to the flow via appropriate heat and mass transfer coefficients. The model neglects axial conduction in both the gas and in the solid. The model includes both detailed gas-phase reactions and catalytic surface reactions. The reactants modeled so far include lean mixtures of dry CO and CO/H ₂ mixtures, with pure oxygen as the oxidizer. The results include transient computations of light-off and system response to inlet condition variations. In some cases, the model predicts two different steady-state solutions depending on whether the channel is initially hot or cold. Additionally, the model suggests that the catalytic ignition of CO/O ₂ mixtures is extremely sensitive to small variations of inlet equivalence ratios and parts per million levels of H ₂ .				
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